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Density matrix averaged atomic natural orbital (ANO) basis sets for correlated molecular wave functions

II. Second row atoms

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Summary. Generally contracted basis sets for second row atoms have been constructed using the Atomic Natural Orbital (ANO) approach, with modifications for allowing symmetry breaking and state averaging. The ANOs are constructed by averaging over several atomic states, positive and negative ions, and atoms in an external electric field. The contracted basis sets give virtually identical results as the corresponding uncontracted sets for the atomic properties, which they have been designed to reproduce. The design objective has been to describe the ionization potential, the electron affinity, and the polarizability as accurately as possible. The result is a set of well balanced basis sets for molecular calculations. The starting primitive sets are $17s12p5d4f$ for the second row atoms Na–Ar. Corresponding ANO basis sets for first row atoms have recently been published.

Key words: ANO – Correlated molecular wave functions – Second row atoms – Ionization potential – Electron affinity – Polarizability

1. Introduction

Density matrix averaged Atomic Natural Orbital (ANO) basis sets [1] for the first row atoms H–Ne have recently been published [2]. The contraction coefficients in these basis sets were obtained by computing the natural orbitals from an averaged density matrix. Singles and doubles configuration interaction (SDCI) were performed for the atom in its ground state, the positive and negative ions, and the ground state atom placed in a small homogeneous electric field. In some cases excited atomic states were also included. The final density matrix used to construct the ANOs was obtained as the average of the density matrices obtained from these SDCI wave functions. The resulting ANOs give simultaneously accurate values for the ionization energy, the electron affinity, and the polarizability of the atoms. The truncation errors for these properties were found to be very small. A number of calculations on small and medium-sized molecules have been performed and show that accurate results can be obtained with these ANO basis sets.

We present here corresponding basis sets for the second row atoms Na–Ar. To our knowledge no compilation of ANO basis sets for second row atoms have hitherto been published. Such basis sets have, however been used in a number of applications (see for example Ref. [3]). The basis sets compiled here have been devised in the same way, as was done for the corresponding basis sets for first row atoms [2]. The size has been chosen such that the same level of accuracy is obtained. Thus the two basis sets should establish a common, balanced, set of basis functions for calculations on molecules containing first and second row atoms. This line of development will continue to the following rows, but not at present. We feel that the need for smaller ANO-type basis sets, which can be used on larger systems is more urgent. The next papers in this series will therefore compile such basis sets for the atoms H–Kr.

The averaging procedure used to obtain the ANOs follows closely that used for the first row atoms [2] and it will only be briefly discussed here. However, the exponents of the primitive functions were for the second row atoms determined in a different way than was used for most of the first row atom basis sets. This will be discussed in some detail in the next section.

2. The primitive basis set and contraction

The construction of the primitive basis set was carried out in a sequence of steps. In the first step the exponents of a $16s11p$ set were optimized in SCF calculations on ground state atoms. For Na and Mg the excited states ^2P and $(3s)(3p)\ ^3P$, respectively, were used in the optimization of the exponents for the p-type functions. The exponents $(\zeta_i, i = 1, n)$ were not individually optimized, but a modified even tempered form [2, 4] was used with three variational parameters $(c_{-1}, c_0$, and $c_1)$:

$$\ln(\zeta_k) = c_{-1}/k + c_0 + c_1 k; \qquad k = 1, \ldots, n; \qquad \zeta_1 > \cdots > \zeta_n \tag{1}$$

which yields energies close to those obtained with individually optimized exponents. Next, four d-type and three f-type functions were optimized in an even tempered form with respect to the valence SDCI energy of the ground state of the atom. Such a procedure could obviously not be used for the Na atom. Instead the optimization was performed on the Na_2 molecule. The optimized primitive sets were augmented with one diffuse function for each angular type. The exponents for these functions were taken as 0.4 times the smallest exponents of the $16s11p4d3f$ sets. The resulting primitive basis sets have the size $17s12p5d4f$. The corresponding ground state Hartree–Fock (HF) energies deviate from numerical HF energies [5] with less than 1.0 mH, except for Ar where the difference is 1.4 mH. These energies are given in Table 1. For S and Cl the present energies are lower than the numerical HF energies, because full spherical symmetry has not been imposed here.

The final ANOs were derived from the average density matrix obtained through SDCI calculations on the atoms (in the case of Na also on the diatomic molecule), positive and negative ions, and on the atoms in a homogeneous electric field. The different SDCI wave functions used to build the average density matrix are shown in Table 2.

These basis sets can be truncated at will. However, below we shall show some results obtained using the truncations $6s5p4d3f$, $5s4p3d2f$, and $4s3p2d1f$. These basis sets should be well balanced with the corresponding first row ANOs

Table 1. Ground state atom SCF, SDCI, and numerical HF energies[a] from the primitive 17*s*12*p*5*d*4*f* basis set

Atom	Numerical HF[a]	SCF	SDCI
Na(^2S)	−161.85891	−161.858209	—
Mg(^1S)	−199.61463	−199.613956	−199.647899
Al(^2P)	−241.87671	−241.876086	−241.931674
Si(^3P)	−288.85436	−288.853694	−288.933737
P(^4S)	−340.71878	−340.717851	−340.822100
S(^3P)	−397.50490	−397.506138	−397.652961
Cl(^2P)	−459.48207	−459.482660	−459.671182
Ar(^1S)	−526.81751	−526.816050	−527.043507

[a] Ref. [5]

Table 2. Wave functions from which the average density matrix have been constructed

State	Na	Mg	Al	Si	P	S	Cl	Ar
Ground state	yes	yes	yes	yes	yes	yes	yes	yes
Molecule	yes	no	no	no	no	no	no	no
Cation	yes	yes	yes	yes	yes	yes	yes	no
Anion	yes	no	yes	yes	yes	yes	yes	no
Field = 0.01 a.u.	yes	yes	no	no	no	no	no	no
Field = 0.02 a.u.	no	no	yes	no	no	no	no	no
Field = 0.05 a.u.	no	no	no	yes	yes	yes	yes	yes

Table 3. The electron affinities (in eV) of the ground state atoms Na–Ar computed using an SDCI wave function

Basis	Na	Mg	Al	Si	P	S	Cl	Ar
primitive	0.541	<0	0.361	1.318	0.395	1.740	3.315	<0
6*s*5*p*4*d*3*f*	0.540	<0	0.358	1.318	0.390	1.738	3.315	<0
5*s*4*p*3*d*2*f*	0.542	<0	0.359	1.315	0.379	1.731	3.311	<0
4*s*3*p*2*d*1*f*	0.539	<0	0.349	1.314	0.337	1.684	3.266	<0
exp[a]	0.548	<0	0.441	1.385	0.747	2.077	3.617	<0

[a] Experimental results from Ref. [6]

containing one function less in each shell. It should be emphasized that the present basis sets have been obtained from calculations of the valence correlation energy. The 1*s* through 2*p* atomic orbitals are described by only one contracted function each. Such a basis set cannot be used to treat core-core or core-valence correlation effects.

3. Test calculations

The basis sets presented here have been designed to be good general purpose basis sets for molecular calculations with primitive sets, that are not prohibitively large for sizeable molecules. Some of the flexibility in the basis sets is inevitably

Table 4. The ionization potentials (in eV) of the ground state atoms Na–Ar computed using an SDCI wave function

Basis	Na	Mg	Al	Si	P	S	Cl	Ar
primitive	4.951	7.532	5.917	8.080	10.436	9.997	12.636	15.487
6s5p4d3f	4.951	7.531	5.916	8.080	10.439	9.995	12.634	15.503
5s4p3d2f	4.949	7.531	5.906	8.071	10.438	9.980	12.621	15.563
4s3p2d1f	4.950	7.524	5.903	8.062	10.393	9.909	12.612	15.654
exp[a]	5.14	7.64	5.98	8.15	10.98	10.36	13.01	15.755

[a] Experimental results from Ref. [7]

Table 5. The average polarizability (in au) of the ground state atoms Na–Ar computed using an SDCI wave function

Basis	Na	Mg	Al	Si	P	S	Cl	Ar
primitive	202.2	75.88	59.75	37.56	24.97	19.27	14.47	11.00
6s5p4d3f	202.4	75.73	59.27	37.39	24.86	19.26	14.47	10.94
5s4p3d2f	203.0	75.57	58.12	36.75	24.85	19.47	14.37	10.92
4s3p2d1f	203.0	75.27	57.18	36.17	25.35	18.81	12.40	8.58
Ref. 8	192.8	75.81	57.47	36.70	24.68	19.60	14.71	11.10
exp[a]	159.2	—	—	—	—	—	—	11.07

[a] Experimental results from Ref. [9] (Na) and [10] (Ar)

lost when they are contracted and truncation errors occur. Tables 3–5 show how the electron affinity (EA), the ionization potential (IP), and the polarizability is affected by truncation at different levels. All properties are calculated at the SDCI level except for the one-electron cases, which are described by an open shell SCF wave function. Correlation is for valence electrons only and no core-core or core-valence correlation effects have been included.

The effect of truncation is negligibly small for the basis sets *6s5p4d3p* and *5s4p3d2f*. Also the smallest basis set tested here, *4s3p2d1f*, yields small errors for the ionization energies and electron affinities, compared to the results obtained with the primitive basis set. The polarizabilities are somewhat more affected, however, indicating the need for more diffuse polarization functions for this property. The results for the polarizabilities in Table 5 are also compared to the Valence CEPA results reported by Reinsch and Meyer [8], which have been obtained using a *14s11p4d* basis sets. As can be seen the differences are small, except maybe for Na. However the results for Na are contaminated by higher polarizabilities due to the use of a too large electric field (0.01 a.u.) in the finite field calculations. The calculations for this atom have therefore been repeated with a smaller field, (0.001 a.u.). At the same time a more careful check of the basis set dependence has been carried out by adding more diffuse primitives to the basis set. This has been done in an even tempered fashion with the coefficient 0.4. The results are presented in Table 6. It is clear from these results that a further extension of the basis set will have no effect on the polarizability.

Experimental data have also been included in Tables 3–5. In comparing the calculated values to experiment one must, however, take into account that the calculations have been performed at the SDCI level of approximation with correlation of only the valence electrons. Two important correlation effects are

Table 6. Polarizability of the sodium atom computed with different primitive and ANO basis sets, using the finite field method and a field of 0.001 au

Basis set	Energy ($F = 0.0$ au)	Energy ($F = 0.001$ au)	Polarizability
17s12p	−161.85820946	−161.85830387	188.82
18s13p	−161.85820983	−161.85830423	188.80
17s12p5d	−161.85820946	−161.85830470	190.48
17s12p6d	−161.85820946	−161.85830470	190.48
17s12p5d4f	−161.85820946	−161.95930470	190.48
ANO *6s5p*	−161.85820931	−161.85830365	188.68
ANO *6s5p4d*	−161.85820931	−161.85830434	190.06
ANO *6s5p4d3f*	−161.85820931	−161.85830434	190.06

Table 7. Cluster corrections to the electron affinity and ionization potential of the sulphur atom obtained with the *5s4p3d2f* ANO basis set

Method	EA (eV)	IP (eV)
SCF	0.90	9.09
SDCI	1.73	9.98
SDCI + Q	1.87	10.08
CPF	1.85	10.06
exp.	2.08^{a}	10.36^{b}

^{a} Ref. [6]; ^{b} Ref. [7]

thus missing: core-valence correlation and cluster corrections to the valence electron correlation energy. The first effect dominates the error for the lighter elements with few valence electrons, while the cluster effects become important especially for S, Cl, and Ar. The cluster corrections to the EA and IP were investigated for the sulphur atom with the *5s4p3d2f* basis set. SDCI and CPF [11] calculations were performed and the cluster corrections to the SDCI energies (SDCI + Q) were obtained using the Davidson method [12]. The results are presented in Table 7.

The cluster corrections to the EA is 0.13 eV if the SDCI + Q energies are used. Almost the same correction is found with the CPF method. Adding this correction gives a total EA, which deviates from experiment with 0.20 eV. A similar error was in the first paper in this series reported for the EA of the oxygen atom. In both cases the error is most certainly due to limitations in the primitive basis set, mainly lack of higher angular momentum functions. The same situation obtains for the IP where the SDCI + Q error is 0.28 eV with the present basis set. Both these discrepancies must be considered satisfactory, considering the limited number of higher angular momentum functions included in the present basis set.

In order to further check the basis set errors for the EA and IP, we have also made calculations on $S^{+}(^{4}S)$, $S(^{3}P)$, and $S^{-}(^{2}P)$ using numerical orbitals. These calculations were performed using the Restricted Active Space (RAS) SCF method [13]. A program for atomic RASSCF calculations with numerical orbitals was used [14]. A HF calculation on $S(^{3}P)$ was first carried out. The *1s*, *2s*, *2p*, *3s*, and *3p* orbitals determined at this level were left frozen in the

RASSCF calculation. The RASSCF wave function had the neon shell inactive. The RAS2 space contained the sulphur 3*s* and 3*p* orbitals. One or two electrons were allowed to excite from these orbitals into 4*s*, 4*p*, 3*d*, 4*d* or 4*f* orbitals. These orbitals constitute the RAS3 space. The wave function is thus of SDCI type. The RAS3 orbitals were determined together with the CI expansion coefficients in the RASSCF optimization procedure. These calculations gave an IP of 9.92 eV and an EA of 1.61 eV, to be compared to 9.91 and 1.68 eV, respectively, obtained with the present 4*s*3*p*2*d*1*f* basis set. The good agreement shows that the present orbitals are well described by the primitive functions used.

It is well known that ANO basis sets give only small errors due to basis set superposition (BSSE) [3] for first row atoms. In order to investigate the BSSE for the present second row orbitals we have made calculations on the chlorine atom with a set of chlorine ghost orbitals located at a distance of 3.76 au from the atom (corresponding to the equilibrium bond distance in Cl_2). The computed SDCI superposition errors for the 6*s*5*p*3*d*2*f*, 5*s*4*p*3*d*2*f*, and 4*s*3*p*2*d*1*f* basis sets were 0.110, 0.120 and 0.192 eV, respectively. The corresponding BSSEs on the SCF level were much smaller: 0.0013, 0.0027, and 0.0115 eV, respectively. In order to investigate how much higher angular momentum functions contribute to the BSSE on the SDCI level, we have repeated the calculations with one *g*-type GTO added to the 5*s*4*p*3*d*2*f* basis set. The exponent used was 0.79. This amendment to the basis set reduces the SDCI BSSE from 0.120 to 0.066 eV. It is thus clear that most of the superposition error obtained with the present basis sets is due to missing basis functions with higher angular momentum.

4. The P_2 and MgS molecules

As a first test of the quality of the present basis sets we have chosen to study the potential curves for the ground state of the two molecules P_2 and MgS. P_2 is a covalently bonded molecule with a relatively strong bond, while MgS is highly ionic. The two sets of calculations will therefore test different qualities of the basis sets. The two smaller ANO sets, 5*s*4*p*3*d*2*f* and 4*s*3*p*2*d*1*f* have been used. The calculations were performed with the MOLCAS-1 quantum chemistry software package [17].

A. The P_2 *molecule*

The P_2 molecule was treated using the CASSCF [15] and MRCI approach [16]. The CASSCF calculations had the neon core orbitals inactive. The active orbitals were those which could be constructed from the 3*s* and 3*p* atomic orbitals. The MRCI wave function was of the second order CI (SOCI) type. Thus all configurations of the CAS wave function were included in the reference space. No excitations from the core orbitals were included in the MRCI wave function in this first set of calculations.

The results from this study are presented in Table 8. The first striking feature of these results is the small difference between the values obtained with the small and large basis set, respectively. The calculated dissociation energy is almost the same. The only improvement comes in the bond distance, which is shortened with 0.01 Å on the MRCI + Q level of treatment. If only CASSCF calculations are to be performed, there is clearly no need to extend the basis set beyond

Table 8. Calculated and experimental spectroscopic constants for the P_2 molecule

	R_e (Å)	D_e (eV)	ω_e (cm^{-1})	$\omega_e x_e$ (cm^{-1})	B_e (cm^{-1})
4s3p2d1f					
CASSCF	1.926	4.18	757	2.55	0.293
MRCI	1.026	4.66	757	2.61	0.293
MCRCI + Q	1.930	4.69	749	2.23	0.292
5s4p3d2f					
CASSCF	1.925	4.14	755	2.73	0.294
MRCI	1.918	4.66	762	4.35	0.296
MRCI + Q	1.921	4.71	755	3.69	0.295
4s3p2d1f + *1s1p1d* (core-valence)					
CASSCF	1.922	3.91	748	—	0.295
MRCI	1.912	4.64	757	—	0.298
MRCI + Q	1.914	4.72	754	—	0.298
exp.[a]	1.893	5.08	781	2.84	0.303

[a] Ref. [18]

4s3p2d1f. The second striking feature of the results obtained for the P_2 molecule is the relatively large differences between the computed and experimental parameters. The calculated bond distance is with the larger basis set 0.028 Å longer than the experimental value and the dissociation energy is 0.37 eV too small. The large error on the computed bond distance is unusual for a calculation at the present level of sophistication. It is not likely that these results can be largely improved by extending the basis set further. Instead other sources for the error have to be found. One possible candidate is core-valence correlation, which has recently been shown to give a non-negligible contribution to the computed bond distance in the PH_3BH_3 molecule [19]. The bond distance was shortened with more than 0.01 Å, when the MRCI wave function was amended with core-valence double excitations. A similar, and probably larger effect can be expected for the P_2 molecule. In order to study this effect it is necessary to add to the basis set functions in the core-valence region. A preliminary investigation of the core-valence correlation effects on the spectroscopic constants in P_2 has been performed. The necessary amendment of the basis set was achieved by performing two sets of SDCI calculations on the phosphorous atom using the *primitive* basis set. In one calculation only the valence electrons were correlated. The CI space was increased in the second calculation by adding all configurations with one hole in the (*2s2p*) shell. A comparison of the natural orbitals from the two calculations showed that it was possible to identify one *s*-type, one *p*-type, and one *d*-type orbital which carried most of the core-valence correlation. These ANOs were added to the *4s3p2d1f* basis set for P_2. The same MRCI calculations as above were then performed, but now adding also all configurations with one hole in the (*2s2p*) core regions. The resulting spectroscopic constants are reported in Table 8. At the CASSCF level only a minor change in the bond distance is obtained. This is gratifying, since it means that the static core polarization is adequately described by the original basis set [20]. At the MRCI level the bond distance is shortened with 0.014 Å. When the effect of increasing the basis set to *5s4p3d2f* is added, a bond distance of 1.904 Å is predicted. Adding the effect of static polarization of the core [20] reduces the distance further to 1.900 Å, which is now only 0.007 Å longer than the experimental value. It should be noted, that we have probably not been able to recover all of the core valence effect on the bond distance with the limited increase of the basis set. The present approach has also a rather limited applicability, since it easily leads to prohibitively large MRCI expansions. The dynamic core polarization is probably better modelled using an effective core polarization operator [21]. The present study does, however, show that it is necessary to include such effects in accurate studies of the structure of molecules containing atoms of the second (or higher) row. The other spectroscopic constants do not change to any appreciable extent with the inclusion of core-valence correlation terms in the wave function. A more detailed account of the calculations on the P_2 molecule will be presented elsewhere.

B. The MgS *molecule*

As a second illustration of the behaviour of the present ANO basis set we have studied the potential curve for the ground state of the MgS molecule. The theoretical determination of the dissociation energies for the alkaline-earth monosulphides is known to be a challenging task due to the large ionic character of these molecules [22]. It has been recommended to compute the dissociation energy of these ionic systems by a combination of theoretical and experimental data. The dissociation to the ionic limits is first computed. In this way the molecular extra correlation energy is expected to be small and recoverable by the calculation. Empirical data for the ionization energy and electron affinity of the separated atoms are then used to obtain the final dissociation energy [22]. This approach has been tested here using MRCI wave functions for the molecule by performing calculations both to neutral and to ionic dissociation limits.

The calculations for the neutral dissociation path were set up similarly to those for P_2. CASSCF calculations were performed first, using an active space comprising the $3s$ and $3p$ shell of the Mg and S atoms. SOCI calculations were then performed based on these reference configurations. The $^1\Sigma^+$ ground state of MgS dissociates to $S(^1D) + Mg(^1S)$. The energy separation between the excited and ground state of the sulphur atom was computed using the same type of wave function as was used for the molecules ($3s$, $3p$ CASSCF and SOCI). The error in the computed energy difference varied from 0.23 eV (CASSCF) to 0.04 eV (MRCI + Q). No attempt was made in this study to include the effect of dynamic core polarization. Thus we expect to obtain a too large bond distance, but if the results on P_2 can be extrapolated, only small effects on the other spectroscopic parameters.

The ionic dissociation limit was obtained by computing also the energies of Mg^+ and S^- using the same methods and basis sets. This essentially means an SCF calculation for Mg^+ and a single reference SDCI calculation for S^-.

The results of the study of the dissociation energy and spectroscopic constants for MgS are compiled in Table 9. Again we see that the small $4s3p2d1f$ basis already gives results rather close to the bigger basis set. The computed bond distance is about 0.03 Å too long at the MRCI level with the larger basis set. The smaller basis set yields a value 0.007 Å longer. Most of this error is due to the lack of core-valence correlation in the wave function. The computed dissociation energy for direct dissociation is 2.21 eV (MRCI + Q) with the large basis set and 2.25 eV with the smaller. These values are actually rather close to

Table 9. Calculated and experimental spectroscopic constants for the MgS molecule

	R_e (Å)	D_e (eV)[a]	D'_e (eV)[b]	ω_e (cm^{-1})	B_e (cm^{-1})	μ (D)[d]
4s3p2d1f						
CASSCF	2.181	1.61 (1.82)	2.59	471	0.254	2.83
MRCI	2.177	2.15 (2.21)	2.40	504	0.259	2.84
MRCI + Q	2.179	2.25 (2.29)	2.39	504	0.259	—
5s4p3d2f						
CASSCF	2.179	1.60 (1.83)	2.57	498	0.259	2.83
MRCI	2.170	2.10 (2.16)	2.34	504	0.260	2.85
MRCI + Q	2.172	2.21 (2.24)	2.32	503	0.260	—
exp.[d]	2.142	$\leqslant$2.4	$\leqslant$2.4	529	0.268	—

[a] Dissociation to ground state atoms. The $S^{-1}D-{}^3P$ separation has been computed at the same level of accuracy. Values within parentheses have been obtained by using instead the experimental value (1.145 eV) for this separation

[b] Computed dissociation to the ionic limit. Ground state dissociation limit obtained using experimental values for the *IP* of Mg (7.644 eV [7]) and the electron affinity of S (2.077 eV [6])

[c] Dipole moment computed at the experimental internuclear distance, 2.142 Å

[d] Ref. [18]

the result obtained using the ionic dissociation path, 2.39 and 2.32 eV, respectively, which shows that the molecular extra correlation energy is recovered to a large extent also along the neutral dissociation path. The value 2.32 eV obtained from the empirically corrected ionic dissociation is on the other hand in excellent agreement with the value, 2.32 ± 0.15 recommended by Partride et al. [22].

The dipole moment was also computed. The value obtained is almost the same with both basis sets and is only to a minor degree affected by the dynamic correlation effects. To our knowledge there is no experimental value for the dipole moment of MgS. Recently, Fowler and Sadlej have computed it using fourth order many-body perturbation theory and a segmented CGTO basis set (*13s10p4d* contracted to *7s5p2d*). The value 2.82 D is obtained in close agreement with the present results [23].

5. Conclusions

The basis sets given in the appendix of the present contribution have been obtained by an averaging procedure, which includes electronic states of the atom, which are important in chemical bond formation. Thus, the orbitals have been constructed such that they simultaneously give accurate values for the ionization potential, the electron affinity, and the polarizability of the atom. Results for these properties that are stable with respect to basis set truncation have also been obtained. It is clear from the test calculations on small molecules that the truncation errors are also small for the molecular properties. Like other ANO basis sets, the present set has the additional virtue of yielding only small basis set superposition energies, which is important, especially when they are used to calculate intermolecular forces. It is also clear from the test calculations performed on P_2 and MgS that very accurate results for molecules containing second row atoms can only be obtained with the inclusion of core-valence correlation effects. This is obviously not a new conclusion since it is confirmed by a number of data from the literature.

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Appendix

The contracted ANO basis functions for the atoms Na to Ar are given in this appendix. For every atom the largest contracted basis set is given: $7s6p4d3f$. These basis sets can be further contracted by just deleting functions from the right. The weakly occupied ANOs contain a mixture of correlation and polarization effects. Thus, when only one orbital is used, a compromise between polarization and correlation is obtained. The major contribution to both these features is obtained with two orbitals. The smallest recommended basis set to be used with these ANOs is $4s3p2d$, which is of double zeta quality in the valence region. Larger basis sets will include more of the finer details in polarization and correlation. Basis sets of the quality $5s4p3d2f$ will give results close to the uncontracted limit.

The basis sets can be made available from the authors, either on a diskette, or through electronic mail (IBMPOW at SEHELIOS).

Sodium atom

Exponent	1s	2s	3s	4s	5s	6s	7s
138773.72	.00007636	-.0000187	.00000255	-.0000023	.00000364	-.0000017	.00000819
20325.899	.00052939	-.0001291	.00001760	-.0000160	.00002582	-.0000100	.00005880
5878.6049	.00183722	-.0004511	.00006160	-.0000553	.00008615	-.0000489	.00018769
2015.4373	.00653431	-.0015982	.00021769	-.0001986	.00032753	-.0001277	.00072363
739.62658	.02092231	-.0052135	.00071184	-.0006340	.00100249	-.0007775	.00191318
280.82116	.06426610	-.0162727	.00221369	-.0019971	.00347727	-.0027220	.00553738
108.71501	.17089923	-.0464583	.00632867	-.0054659	.00977528	-.0168111	.00451727
42.601572	.35610342	-.1114445	.01509121	-.0127624	.02880208	-.0709184	-.0286277
16.829817	.40213461	-.1853734	.02530901	-.0187696	.05266945	-.2394172	-.2003790
6.6864486	.12746393	-.0600544	.00808949	-.0074755	.02852077	-.0608347	-.0460225
2.6674877	.00061064	.35924086	-.0530507	.03897469	-.1812429	.78439608	.73703463
1.0674621	.00338457	.57207971	-.1116411	.08327536	-.1468356	.84719710	.54990865
.42818910	-.0013287	.22321420	-.1383134	.20560497	-.3398427	-2.036253	-4.055087
.17208010	.00085748	-.0050286	-.0299010	-.0468315	.65955083	-.2422682	6.8456427
.06925880	-.0004761	.00595957	.44900485	-.7982314	1.8591377	2.3580377	-6.673005
.02790920	.00022186	-.0025377	.47484493	-.5759529	-3.557612	-2.255780	4.1780972
.01116330	-.0000638	.00078635	.22905052	1.4408654	1.8865531	.90445966	-1.377566

Exponent	2p	3p	4p	5p	6p	7p
383.79172	.00102867	-.0001186	.00015162	-.0001858	.00002038	-.0005510
94.398072	.00743093	-.0008634	.00110681	-.0011546	-.0004979	-.0029822
32.361507	.03273646	-.0037997	.00487773	-.0060608	.00196514	-.0176344
12.054352	.11687036	-.0138426	.01792042	-.0182851	-.0008732	-.0411126
4.6417186	.27753763	-.0331504	.04350073	-.0559810	.05166830	-.1682873
1.8172876	.39800015	-.0489974	.06554272	-.0567200	-.0102429	-.0883103
.71827120	.32331086	-.0465827	.07245938	-.1506721	.47624183	-.6810114
.28558030	.09433492	-.0302457	.09073829	-.0033550	-.8897463	2.7426269
.11399470	.00109373	.22294313	-.7676374	1.5488268	-.2605509	-3.415643
.04562920	.00178158	.50923252	-.3977149	-1.899464	1.9011944	2.8918651
.01830100	-.0006980	.37196823	.92303779	.39892154	-2.634481	-1.952736
.00732040	.00022539	.04475107	.17065606	.64929030	1.6808822	.83260624

Exponent	3d	4d	5d	6d
.86260360	.02177426	-.0134860	.02840092	-.2199697
.34514180	-.0072186	-.0029987	-.2061890	-1.328911
.13809690	.33517471	-.4666753	-1.215883	1.7464842
.05525480	.36379749	-.6237490	1.8313353	-1.181551
.02210190	.49254995	1.1090949	-.9208703	.45691840

Exponent	4f	5f	6f
.32814490	.01063271	-.0383335	.14999444
.15734730	-.4959911	-.3009833	1.3496919
.07544890	-.2628732	-.6460291	-1.836927
.03017960	-.4748596	1.1242100	.72136130

Magnesium atom

Exponent	1s	2s	3s	4s	5s	6s	7s
169973.87	.00007417	-.0000188	.00000379	-.0000044	.00000684	-.0000071	.00001321
24699.066	.00051736	-.0001306	.00002638	-.0000308	.00004631	-.0000421	.00007728
7175.4851	.00177276	-.0004501	.00009109	-.0001046	.00016849	-.0001922	.00036299
2478.7920	.00623864	-.0015794	.00031906	-.0003749	.00054725	-.0004400	.00079337
917.73259	.01976587	-.0050907	.00103163	-.0011803	.00193137	-.0022980	.00436287
351.75140	.06017463	-.0157521	.00318903	-.0037548	.00545737	-.0042807	.00776087
137.51557	.16016295	-.0448403	.00913931	-.0104620	.01729461	-.0210084	.04052022
54.430286	.33917581	-.1085387	.02227591	-.0263896	.03812473	-.0284298	.05182257
21.722569	.40883352	-.1875980	.03965557	-.0450679	.07914147	-.1087140	.21014157
8.7194484	.15183413	-.0868386	.01868253	-.0255703	.01594961	.06640619	-.1568166
3.5147166	.00195927	.33464216	-.0800164	.10765675	-.1396824	-.0173897	-.0205122
1.4212132	.00418518	.59813818	-.1882757	.21164824	-.5343596	1.1451315	-2.332119
.57607650	-.0018766	.23180428	-.2116262	.43129749	-.2813320	-1.776326	5.8896808
.23395250	.00120338	-.0069386	.14066560	-.9682371	3.0868468	-.1236407	-7.260361
.09515600	-.0006745	.00680179	.68477064	-.9734396	-3.537601	3.0022439	6.3580954
.03875100	.00031460	-.0028030	.34545022	1.4680586	1.0258502	-4.229333	-4.170206
.01550040	-.0000888	.00083003	.00874972	.09800990	.56587909	2.4153747	1.5689747

Exponent	2p	3p	4p	5p	6p	7p
557.13078	.00079833	-.0001612	.00013230	-.0002160	.00031544	-.0003802
135.48388	.00589231	-.0011931	.00094881	-.0004842	.00072367	-.0104720
47.212958	.02583591	-.0052464	.00431193	-.0075094	.01089367	-.0108832
18.000955	.09406296	-.0193118	.01513244	-.0037304	.00243732	-.2138345
7.1146607	.24134480	-.0504945	.04187188	-.0798884	.12540044	-.0110486
2.8630240	.38746464	-.0829628	.06595574	.01126479	.01067632	-1.288154
1.1640185	.35595067	-.0882749	.09294055	-.5605788	1.0932302	2.6093729
.47630470	.12288168	-.0397079	.05017503	.66659154	-3.222922	-1.912959
.19573560	.00380787	.42165449	-.7562222	1.2375291	3.6486214	.65864915
.08067830	.00230283	.58978450	-.1812787	-2.367450	-2.391198	.46088594
.03332660	-.0008589	.10380275	1.0389702	1.2973603	.71760597	-1.195422
.01333060	.00027579	.00502440	.09524704	.07151495	.17597721	.94673660

Exponent	3d	4d	5d	6d
1.0445644	.01605667	-.0428969	.20912538	-.1492952
.48574730	.02264646	.18907793	-.9043652	2.1174840
.22588410	.46449386	.77129122	-.2945459	-3.252542
.10504150	.47219231	-.3211997	1.5734652	2.4351200
.04201660	.16336646	-.7606902	-1.168275	-.9326178

Exponent	4f	5f	6f
.49952380	.00588707	-.3040746	1.3305087
.28386680	-.5119605	-1.113993	-1.052751
.16131440	-.4697872	1.1067098	-.4877023
.06452580	-.1174511	.30597008	.97122301

Aluminium atom

Exponent	1s	2s	3s	4s	5s	6s	7s
208459.49	.00007078	-.0000184	.00000432	-.0000043	.00000648	-.0000078	.00001478
29971.598	.00049759	-.0001292	.00003029	-.0000305	.00004502	-.0000473	.00008690
8764.4565	.00167444	-.0004371	.00010265	-.0001022	.00015532	-.0002100	.00040482
3060.7073	.00580246	-.0015120	.00035421	-.0003589	.00052217	-.0004756	.00084713
1147.4963	.01811648	-.0047943	.00112743	-.0011192	.00171468	-.0024397	.00474942
445.75595	.05440537	-.0146291	.00343446	-.0034867	.00506469	-.0044616	.00796079
176.70642	.14492054	-.0414399	.00980341	-.0097405	.01501684	-.0217738	.04310749
70.943620	.31321200	-.1011887	.02408671	-.0245903	.03577722	-.0301325	.05458496
28.724000	.41334250	-.1844770	.04527494	-.0449818	.07132737	-.1175912	.24022746
11.698923	.19059653	-.1227370	.03095121	-.0340410	.04282415	.04163135	-.1294530
4.7853697	.00707487	.27348316	-.0757518	.08910950	-.1335589	-.0325805	-.0726848
1.9637518	.00484032	.61530733	-.2248045	.22809994	-.4448498	1.2270504	-2.487643
.80785940	-.0023301	.28146024	-.2548542	.38525013	-.5214934	-1.450690	6.2559149
.33299060	.00153518	-.0050360	.20149503	-.8008886	2.9480591	-1.201880	-7.656582
.13746930	-.0008688	.00796206	.68310534	-.9996260	-2.576996	4.2755051	6.5506643
.05682380	.00040223	-.0035364	.30782923	1.1980110	-.1936730	-4.778359	-4.069422
.02272950	-.0001112	.00100247	.02408008	.36451428	1.1061036	2.3292396	1.4181068

Exponent	2p	3p	4p	5p	6p	7p
677.76458	.00079717	-.0001373	.00015515	-.0001686	.00036347	-.0004317
164.83442	.00589941	-.0010123	.00113147	-.0010857	.00162437	-.0044732
57.683424	.02586307	-.0044952	.00508163	-.0055883	.01256209	-.0139014
22.108674	.09471373	-.0165714	.01841598	-.0171321	.02439129	-.0756068
8.7877514	.24484796	-.0441449	.05014804	-.0562246	.13515491	-.1483713
3.5570874	.39837993	-.0724803	.08138367	-.0722489	.06998835	-.3840019
1.4548780	.35294610	-.0746550	.09799899	-.1696058	.56219989	.12941033
.59893630	.10280005	.01880214	-.0184402	.10547020	-1.547522	1.8975640
.24763730	.00234580	.27739515	-.6277481	1.0958721	.33806270	-3.448842
.10269950	.00175805	.44207475	-.2459852	-.8023042	1.6903272	3.6086484
.04268530	-.0005341	.29055057	.35129892	-.9238459	-2.215065	-2.574987
.01707410	.00019528	.16625332	.65543563	1.1608148	1.1012016	1.0063049

Exponent	3d	4d	5d	6d
1.2673144	.01856849	-.0067653	.15132202	-.0839790
.50951300	.11745821	.20578256	-.9059657	1.5088184
.20484530	.50149748	.54053298	-.0459154	-2.329156
.08235630	.37968233	-.0892098	1.2672360	1.9665618
.03294250	.20021391	-.8711067	-.9817175	-.8938278

Exponent	4f	5f	6f
.56231110	.08418120	-.2078943	.67102451
.27076610	.45945383	-.4049650	.44008697
.13038030	.38017523	-.1752296	-1.416253
.05215210	.29286740	.97536728	.84507591

Silicon atom

Exponent	1s	2s	3s	4s	5s	6s	7s
250095.97	.00006815	-.0000182	.00000470	-.0000049	.00000688	-.0000087	.00001467
35803.200	.00048017	-.0001278	.00003305	-.0000348	.00004735	-.0000518	.00008792
10522.483	.00159626	-.0004265	.00011064	-.0001149	.00016522	-.0002376	.00039439
3701.7745	.00547507	-.0014618	.00037778	-.0004007	.00053088	-.0004902	.00084912
1399.3933	.01693706	-.0045845	.00119120	-.0012329	.00179852	-.0027360	.00453107
548.38895	.05041784	-.0138701	.00359228	-.0038201	.00503523	-.0044465	.00780858
219.36269	.13450267	-.0391782	.01024273	-.0106138	.01559960	-.0241599	.04050608
88.882259	.29476401	-.0963506	.02530364	-.0270878	.03568620	-.0301527	.05497664
36.323377	.41279726	-.1817620	.04932521	-.0512202	.07863781	-.1375365	.23649293
14.933463	.21885760	-.1452339	.04049616	-.0466301	.04948931	.04506541	-.0821614
6.1663485	.01352631	.22989807	-.0698564	.09190140	-.1113745	-.0723206	-.1205061
2.5545565	.00478761	.62379847	-.2541120	.26901327	-.5522929	1.4944138	-2.468314
1.0609507	-.0023509	.31543582	-.2861133	.46077703	-.3884090	-2.002250	6.3336494
.44150240	.00157700	-.0027626	.24639415	-1.056201	2.9534782	-.5249362	-7.994300
.18401680	-.0009118	.00903722	.68019181	-.7847112	-2.855602	3.7709274	7.0780701
.07679620	.00041644	-.0039062	.28966706	1.2042630	.09215286	-4.557477	-4.503277
.03071850	-.0001140	.00111144	.02414823	.29679859	1.0348260	2.2867174	1.5858588

Exponent	2p	3p	4p	5p	6p	7p
843.53382	.00074369	-.0001574	.00016602	-.0001925	.00040030	-.0004588
204.90726	.00552015	-.0011656	.00119789	-.0011519	.00205111	-.0050227
72.248787	.02411287	-.0051529	.00545750	-.0064766	.01387012	-.0147947
27.961365	.08883573	-.0191723	.01962832	-.0182754	.03298719	-.0887910
11.232282	.23494251	-.0523132	.05586579	-.0680060	.15230781	-.1634705
4.5969373	.39732250	-.0900087	.09197956	-.0775832	.11866287	-.4518247
1.9014833	.36181185	-.0925012	.11503921	-.2143299	.47363973	.42946735
.79178280	.10524773	.03870909	-.0648366	.25572048	-1.683025	1.4690290
.33116620	.00256555	.34152769	-.6831822	1.0777334	.83716261	-3.212659
.13894230	.00177329	.46110561	-.1636095	-1.244684	1.1989226	3.6561945
.05842570	-.0004541	.25855921	.61750164	-.3835503	-2.073387	-2.772948
.02337030	.00017881	.07566560	.44097775	1.0225198	1.1887014	1.1551406

Exponent	3d	4d	5d	6d
2.0105333	.02221051	-.0019527	.13166768	-.2495003
.79109810	.10356980	.15356092	-.6615053	1.7259992
.31127870	.50813164	.48959332	-.4591092	-2.278691
.12248090	.35117535	.11387560	1.5443036	1.7296273
.04899240	.25071127	-.9848990	-.9994450	-.7284053

Exponent	4f	5f	6f
.71849250	.11009981	-.1796744	.65203766
.34744460	.46295659	-.2337503	.54564006
.16801530	.32345259	-.4726389	-1.140904
.06720610	.34355047	1.1086961	.69765331

Phosphorus atom

Exponent	1s	2s	3s	4s	5s	6s	7s
296647.55	.00006562	-.0000178	.00000495	-.0000038	.00000594	-.0000086	.00001571
42380.030	.00046254	-.0001256	.00003483	-.0000268	.00004144	-.0000549	.00009079
12503.856	.00152412	-.0004153	.00011560	-.0000866	.00013959	-.0002171	.00043093
4422.4937	.00518926	-.0014140	.00039175	-.0003050	.00046280	-.0005606	.00081581
1681.8478	.01595159	-.0044003	.00122727	-.0009131	.00148861	-.0024058	.00494091
663.21490	.04720087	-.0132373	.00367506	-.0028728	.00434089	-.0051418	.00724838
267.00585	.12619981	-.0373384	.01047976	-.0077988	.01277688	-.0209076	.04374242
108.89592	.27982529	-.0924440	.02602575	-.0204930	.03096216	-.0361719	.05082520
44.797314	.41030382	-.1790816	.05218594	-.0386560	.06543104	-.1161313	.26661993
18.540312	.24188220	-.1617487	.04842224	-.0419740	.05707014	-.0231251	-.0954873
7.7070995	.02071709	.19399810	-.0627070	.06559604	-.0938614	.01864200	.00792644
3.2143750	.00443622	.62785121	-.2764821	.19549449	-.4100551	1.1215665	-2.949823
1.3440127	-.0021687	.34320722	-.3113284	.38636227	-.4860791	-.6323257	6.9392677
.56308700	.00148760	-.0001020	.27584791	-.7534886	1.9504142	-2.927567	-8.194017
.23628700	-.0008772	.00993085	.67745539	-.5481435	-.2930915	5.8115095	6.6263967
.09928110	.00039698	-.0041808	.28560830	.26985002	-2.307549	-5.021163	-3.715712
.03971240	-.0001079	.00119275	.01675006	.97010724	1.7784766	1.9270723	1.1180021

Exponent	2p	3p	4p	5p	6p	7p
1018.4122	.00071159	-.0001688	.00015264	-.0002211	.00040331	-.0004377
247.39820	.00528387	-.0012501	.00110387	-.0013789	.00219003	-.0050081
87.790482	.02297828	-.0055096	.00500340	-.0074167	.01392847	-.0139403
34.248600	.08494327	-.0205722	.01814153	-.0223634	.03590870	-.0890233
13.877014	.22803285	-.0571783	.05241729	-.0794469	.15612489	-.1605980
5.7303098	.39658377	-.1015364	.08911554	-.1018315	.14452546	-.4724864
2.3920068	.36766734	-.1048700	.10677427	-.2204586	.41344622	.48623525
1.0052767	.10640781	.05753445	-.0721144	.35066535	-1.650833	1.4289213
.42439290	.00281028	.37524649	-.6090964	.97783112	.86123612	-3.298810
.17973060	.00165268	.45668244	-.1615733	-1.121899	1.2175016	3.7980695
.07629100	-.0004011	.22572156	.54191860	-.5059141	-2.115779	-2.824784
.03051640	.00016315	.06188888	.53980064	1.0263412	1.1923436	1.1298443

Exponent	3d	4d	5d	6d
2.7201853	.02567866	-.0128164	.14954306	-.2871423
1.0722222	.12037513	.17873934	-.6658643	1.7664693
.42264050	.55955359	.50423470	-.4006121	-2.302511
.16659330	.37100935	-.1177002	1.5341916	1.7474107
.06663730	.12126366	-.8885982	-1.095009	-.7505496

Exponent	4f	5f	6f
.89440190	.17144038	-.3758042	.76409816
.44087230	.50049572	-.3949707	.06209552
.21731660	.37145759	.26674267	-1.237219
.08692660	.13902900	.76247795	1.0123005

Sulfur atom

Exponent	1s	2s	3s	4s	5s	6s	7s
346348.23	.00006370	-.0000176	.00000516	-.0000038	.00000585	-.0000091	.00001567
49391.146	.00044935	-.0001241	.00003629	-.0000273	.00004096	-.0000571	.00009351
14610.990	.00147142	-.0004076	.00011970	-.0000876	.00013668	-.0002330	.00041879
5187.2095	.00498429	-.0013820	.00040336	-.0003073	.00045296	-.0005625	.00086323
1980.9676	.01525241	-.0042763	.00125841	-.0009151	.00144216	-.0025776	.00472419
784.63139	.04494424	-.0128162	.00374805	-.0028671	.00420970	-.0050685	.00767113
317.32779	.12035338	-.0361097	.01069509	-.0077799	.01231522	-.0223147	.04154294
130.01976	.26908335	-.0898726	.02665475	-.0205390	.03016574	-.0357024	.05501805
53.738208	.40722490	-.1772888	.05454724	-.0395676	.06449660	-.1280024	.25682345
22.345896	.25831856	-.1731201	.05462756	-.0460048	.06268013	-.0214589	-.0404978
9.3332512	.02714669	.16887115	-.0569242	.06098330	-.0876168	-.0189056	-.0715154
3.9111868	.00400872	.63115534	-.2965855	.20575809	-.3943469	1.2906060	-2.897299
1.6432066	-.0019271	.36103178	-.3293273	.40570893	-.5518069	-.8855693	6.9650422
.69174560	.00134644	.00184135	.30470795	-.8189929	1.9999361	-2.714876	-8.363035
.29167360	-.0008115	.01069710	.67383630	-.4447134	-.2782984	5.6893871	6.8878417
.12314410	.00036382	-.0043230	.27748421	.18735812	-2.352825	-4.928902	-3.917652
.04925760	-.0000987	.00124248	.01304772	1.0072258	1.7923271	1.8665411	1.1859567

Exponent	2p	3p	4p	5p	6p	7p
1129.1269	.00077145	-.0001970	.00018333	-.0002800	.00043230	-.0004091
274.03515	.00572945	-.0014624	.00130515	-.0017259	.00288638	-.0061134
97.402584	.02477182	-.0064004	.00600239	-.0094008	.01459323	-.0121902
38.085518	.09109122	-.0238763	.02129088	-.0279784	.04821802	-.1093380
15.471033	.24064577	-.0653201	.06221627	-.1006796	.16282315	-.1401787
6.4056590	.40976882	-.1147693	.09978781	-.1176716	.20594756	-.5829290
2.6812828	.35226804	-.1065702	.11944864	-.2566543	.24014052	1.0378398
1.1300050	.08382797	.11048130	-.1595989	.68243796	-1.826697	.43994605
.47839950	.00271787	.41795827	-.6701145	.66515564	1.8021455	-2.443449
.20318050	.00078655	.42517813	.01331064	-1.445138	.02939534	3.4947292
.08649230	.00011535	.19228231	.64871747	.12745221	-1.469665	-2.985550
.03459690	.00003404	.04207771	.37095119	.77294449	1.1261511	1.3363311

Exponent	3d	4d	5d	6d
3.0053679	.03293922	-.0319187	.15012046	-.1798164
1.2172976	.16386221	.29392107	-.8238332	1.6521729
.49305560	.58677406	.46210890	-.0496411	-2.428826
.19970780	.31916052	-.3236054	1.3217693	1.9779612
.07988310	.08508563	-.7556117	-1.118038	-.8770788

Exponent	4f	5f	6f
1.1000988	.20845644	-.5944200	.91250849
.52721330	.55071337	-.3364989	-.6710704
.25266270	.33354097	.71034940	-.5285472
.10106510	.06724721	.35946202	1.0091990

Clorine atom

Exponent	1s	2s	3s	4s	5s	6s	7s
399432.47	.00006215	-.0000174	.00000531	-.0000047	.00000595	-.0000092	.00001551
56908.833	.00043838	-.0001229	.00003739	-.0000337	.00004122	-.0000559	.00009533
16874.769	.00142781	-.0004013	.00012271	-.0001083	.00013955	-.0002433	.00040362
6010.0278	.00481620	-.0013556	.00041159	-.0003741	.00044686	-.0005185	.00090407
2303.2830	.01468157	-.0041744	.00127960	-.0011233	.00146844	-.0027098	.00447787
915.65994	.04311398	-.0124726	.00379416	-.0034609	.00411004	-.0045562	.00805528
371.72009	.11558388	-.0351047	.01083171	-.0095186	.01251189	-.0234201	.03915746
152.89109	.26016348	-.0877502	.02707379	-.0248663	.02954625	-.0319448	.05872894
63.436303	.40382380	-.1756425	.05631797	-.0496454	.06763368	-.1391522	.24500845
26.481723	.27179877	-.1820699	.05980454	-.0590132	.06396442	-.0053262	.01008609
11.104112	.03338125	.14753370	-.0511335	.06729192	-.0762294	-.0811467	-.1510727
4.6716289	.00356211	.63295111	-.3126721	.26850578	-.4455588	1.4957995	-2.806411
1.9704520	-.0016560	.37614178	-.3437438	.51536265	-.5319150	-1.371860	6.9280066
.83279460	.00117962	.00380802	.32577967	-1.116105	2.3892293	-2.020187	-8.506770
.35254090	-.0007311	.01133746	.66892575	-.5291452	-1.299264	5.2474142	7.2157722
.14943410	.00032425	-.0044445	.27170146	.76655700	-1.504787	-4.985134	-4.249805
.05977360	-.0000879	.00129047	.01386816	.59696595	1.6573777	2.0610818	1.3380072

Exponent	2p	3p	4p	5p	6p	7p
1288.9716	.00078181	-.0002107	.00020575	-.0003172	.00045514	-.0003784
312.24430	.00581729	-.0015704	.00146090	-.0019462	.00362539	-.0069306
111.34634	.02503057	-.0068304	.00673436	-.0106718	.01501985	-.0105414
43.736087	.09188004	-.0255201	.02376316	-.0315749	.06149816	-.1255272
17.856524	.24258072	-.0697489	.07010553	-.1157486	.16963861	-.1251477
7.4327659	.41394424	-.1238756	.11161894	-.1290865	.28532032	-.6700512
3.1282538	.34789086	-.1085162	.12978530	-.2764933	.03758123	1.4960326
1.3257214	.07717314	.13894281	-.2335413	.89183689	-1.854784	-.4868674
.56441910	.00312835	.42954359	-.6718963	.41342424	2.4337684	-1.469269
.24107410	.00050049	.40829131	.10952051	-1.538377	-.9402668	2.9379877
.10320890	.00034786	.18156256	.66424757	.46781029	-.7732962	-2.927422
.04128360	-.0000238	.03396053	.30179468	.59904463	.92109142	1.4598129

Exponent	3d	4d	5d	6d
3.6204561	.03682298	-.0484380	.16746529	-.1146750
1.4775717	.17638808	.39297464	-.9448960	1.5342644
.60302300	.59139283	.47951806	.27892621	-2.416469
.24610430	.30996037	-.5621245	1.0481966	2.0936718
.09844170	.06672018	-.5625776	-1.127109	-1.000086

Exponent	4f	5f	6f
1.3568964	.22438063	-.6873623	1.2894102
.66136460	.56956395	-.2610440	-1.578934
.32235560	.30148671	.82343588	.36185604
.12894220	.04940109	.21671325	.64784529

Argon atom

Exponent	1s	2s	3s	4s	5s	6s	7s
455476.77	.00006096	-.0000173	.00000544	-.0000053	.00000579	-.0000101	.00001574
64817.743	.00043020	-.0001222	.00003829	-.0000375	.00003978	-.0000588	.00010504
19256.987	.00139466	-.0003969	.00012513	-.0001202	.00013641	-.0002726	.00038069
6877.0073	.00468779	-.0013367	.00041795	-.0004134	.00042380	-.0005108	.00108896
2643.4877	.01424066	-.0040986	.00129572	-.0012382	.00143205	-.0030570	.00405999
1054.2375	.04169365	-.0122134	.00382578	-.0037976	.00386068	-.0043637	.00992588
429.37122	.11183053	-.0343322	.01092652	-.0104554	.01216691	-.0263712	.03532764
177.18859	.25298878	-.0861007	.02735689	-.0273526	.02778303	-.0303692	.07413651
73.763945	.40044790	-.1742768	.05765806	-.0554677	.06724781	-.1609503	.22171966
30.897007	.28245090	-.1890266	.06394978	-.0686523	.06200867	.01248080	.11793481
12.999482	.03906305	.13009718	-.0457282	.07055596	-.0604152	-.1543186	-.4561530
5.4876793	.00314565	.63399171	-.3257725	.30115546	-.4638701	1.8359115	-2.314708
2.3225716	-.0013916	.38815020	-.3533104	.61789886	-.4931132	-2.053034	6.4902280
.98498070	.00101034	.00573222	.33817566	-1.433774	2.4139497	-1.208328	-8.429608
.41839730	-.0006485	.01193554	.66223091	-.2709471	-1.535975	4.6352125	7.5075092
.17795940	.00028402	-.0044941	.27636906	.77596409	-1.277294	-4.696117	-4.596645
.07118380	-.0000771	.00131952	.00949692	.50334371	1.6378895	1.9882945	1.4824485

Exponent	2p	3p	4p	5p	6p	7p
1462.4962	.00078756	-.0002212	.00029752	-.0004543	.00038932	-.0004187
354.06731	.00586048	-.0016514	.00201545	-.0031815	.00580901	-.0083769
126.69779	.02510137	-.0071399	.00979652	-.0151158	.01133247	-.0115185
49.989095	.09200774	-.0267171	.03265686	-.0527992	.10360929	-.1567219
20.509295	.24317197	-.0730722	.10366041	-.1702720	.13463887	-.1416172
8.5804641	.41674542	-.1313295	.14799999	-.2312750	.54075660	-.7732953
3.6301049	.34542045	-.1096421	.20744830	-.2035281	-.9562551	2.4202978
1.5465280	.07305360	.16048636	-.5079685	1.7452925	-.5069180	-2.743139
.66193690	.00294397	.43595556	-.8042402	-1.396303	2.3278004	1.6616695
.28424280	-.0002394	.40458441	.69669502	-.4727185	-2.632171	.06039893
.12234630	.00028995	.17125106	.46331690	.89125570	1.0925195	-1.405839
.04893850	-.0000934	.01351308	.04908714	.06889766	.35266723	1.2633622

Exponent	3d	4d	5d	6d
4.3288417	.04003444	-.0575340	.16735357	-.0845008
1.7742302	.18334334	.42320227	-.9667404	1.4950519
.72719060	.59072873	.45075094	.33376377	-2.418135
.29804820	.30437283	-.5696319	1.0041472	2.1173288
.11921930	.06258812	-.5510258	-1.119444	-1.014984

Exponent	4f	5f	6f
1.6311740	.23597497	-.7659268	1.4738938
.82032880	.57618801	-.1737742	-2.048792
.41254910	.27800823	.84810472	.80520996
.16501960	.04019225	.16638315	.46484375